NOTES ON THE VERTICAL GRADIENT INITIALIZATION APPROACH IN THE CPG CFT MODEL IN SUPPORT OF DISCUSSIONS WITH USEPA ON DRAFT LPR RI COMMENTS

During the June 28, 2016 modeling meeting, USEPA Region 2 mentioned the concerns raised in its RI comments regarding discontinuities in the CFT model's initial vertical contaminant concentration profiles for a number of grid cells. Specifically, USEPA Comment No. 556 states: "Attachment 4, Figure 1 shows the vertical profile of initial conditions for a number of grid cells of interest. The first two cells (Figures 1a and 1b) discussed previously in Comment No. 552 have excessive erosion; the next two cells (Figures 1c and 1d) show locations where contaminant concentrations were zeroed at depth; and the final two cells (Figures 1e and 1f) show extremely low concentration discontinuities in the profile of 2,3,7,8-TCDD concentrations. It appears that there is an issue in the vertical interpolation approach presented in this section of the report. Please correct the error that generates these discontinuity errors, revise the text to reflect those corrections, and provide figures displaying the vertical profile used in the model along with the data used to generate the profiles for the locations with discontinuities, locations with erosion in excess of 15 cm, and locations zeroed at depth."

These notes review the application of the vertical gradient initialization approach used to generate the 2,3,7,8-TCDD initial condition (IC) profiles raised in the above comment. The description of the approach from the draft RI report (Appendix O; Section 3.1.2) is provided again for convenience, as the text that follows references the steps described therein:

> This section covers the approach to approximate the vertical concentration structure from 0 to 45 cm; intervals below 45 cm were not adjusted in this regard. The goals of the approach are to: 1) honor the mapped concentrations of the two depth intervals noted above [0-15 cm and 15-45 cm]; 2) ensure a continuous concentration gradient between the intervals when possible; and 3) approximate the 0 to 15 cm shape using the model predictions. A summary of the approach follows:
>
> 1. Development of Subsurface Bed Shape – From 0 to 15 cm, concentrations were set at the measured values as defined by the chemical IC mapping for that interval. A gradient was applied from 15 cm to a depth of 30 cm or less such that a smooth

transition occurred from 15 to 16 cm and the average over the 15 to 45 cm interval matched the measured value (Figure 3-8b).

2. Development of Surface Bed Shape – The concentrations from Step 1 were used as ICs and the model was run through the long-term calibration period (WY1996 to WY2010). The vertical profiles generated by the model over the top 15 cm were then used to re-establish ICs. To do this, the shapes were normalized by the average concentration over the interval to establish a mean-normalized shape (Figure 3-8c).
3. Application of Surface Bed Shape – the mean-normalized shape from the end of the long-term run in Step 2 was applied to the initial sediment concentration to establish a vertical structure for the top 15 cm by multiplying the shape with the value from the surface mapping for the IC of interest (1995 or 2010, as discussed previously) (Figure 3-8d).
4. Redevelopment of Subsurface Bed Shape – A gradient was applied from 15 cm to a depth of 30 cm or less to allow for a continuous concentration profile over the top 45 cm while still honoring the measured values of the 0 to 15 cm and 15 to 45 cm intervals as defined by the chemical IC mapping (Figure 3-8e).

We investigated the vertical concentration profiles raised by USEPA in Comment No. 556 and concluded that the initialization approach is working as designed. The selected profiles reflect one or more of the following effects encountered in the approach:

- Differences between the raw mapped concentrations for the 0 to 15 cm and 15 to 45 cm intervals that are too large to be accommodated by the initialization interpolation function, causing raw IC concentrations from the mapping to remain unadjusted in Step 1.
- Large erosion events during the shape spin-up period (in Step 2) that bring low concentrations from deeper layers into the 0 to 15 cm interval.
- Large deposition events during the shape spin-up period that shift the initial profile downward.
- The time history of more gradual CFT model dynamics (e.g., erosion, deposition, mixing) over the shape spin-up period.

Presented below are detailed descriptions of each step of the initialization process for the selected profiles along with accompanying observations about the bed elevation change.

Figures 1a and 1b of USEPA Attachment 4

The steps to create concentration profiles for grid cells [17, 236] and [17, 234] are shown in Figure 1a and 2a of these notes and the CFT bed thickness changes for the same cells are shown in Figures 1b and 2b (as a surrogate for bed elevation change). The profiles reflect:

Step 0: Raw IC derived from the mapping of sediment core data for each data interval (mapped dry weight concentrations were converted to volumetric concentrations using model bulk density).

Step 1: Subsurface IC for the "shape run". The change in concentration between the 0 to 15 cm and 15 to 45 cm intervals was too large for the interpolation function to accommodate and consequently the raw IC concentration values remained unchanged. The interpolation function is described in detail in Section 3.1.2 of Appendix O of the draft RI report.

Step 2: The concentration profile at the end of the long-term shape run. These cells experienced large erosion events[1] (Figures 1b and 2b), which caused deeper bed layers with low concentrations, some as low as zero[2], to be lifted into the 0 to 15 cm interval. The final shape in the upper 15 cm also reflects more gradual CFT dynamics (e.g., erosion, deposition, mixing) over the remainder of the run.

Steps 3 & 4: Interpolated initial bed concentrations for the model run.

Conclusion: The algorithm is working as designed and the shape is being driven by large erosion events followed by more gradual CFT dynamics during the shape run.

Figures 1c and 1d of USEPA Attachment 4

With regard to USEPA's observation that grid cells [18, 90] and [22, 94] "show locations where contaminant concentrations were zeroed at depth," it is noted that concentrations below 45 cm reflect concentrations set by contaminant mapping[2] and the vertical

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[1] The scour in these cells was noted in USEPA Comment No. 552, and will be evaluated during model revisions.
[2] The mapped concentrations at depth derive from core data and the core data treatment rules described in Appendix O, Section 3.1.1.3.1 of the draft RI report. Note that the 2,3,7,8-TCDD concentrations in this area are low (<1ng/kg).

interpolation algorithm described herein applies only to the upper 45 cm. To address the structure of the upper 45 cm, the steps to create concentration profiles for cells [18, 90] and [22, 94] are shown in Figures 3a and 4a of these notes and the bed thickness changes for the same cells are shown in Figures 3b and 4b. The profiles reflect:

Step 0: Raw IC derived from the mapping of sediment core data for each data interval (converted to volumetric concentration using model bulk density).

Step 1: Subsurface IC for the "shape run". For cell [18, 90], the change in concentration between the 0 to 15 cm and 15 to 45 cm intervals was interpolated to produce a smoother transition in the 15 and 30 cm interval. For cell [22, 94], the change in concentration between the 0 to 15 cm and 15 to 45 cm intervals was too large for the interpolation function (Appendix O, Section 3.1.2) to accommodate and consequently the raw IC concentration values remained unchanged.

Step 2: The concentration profiles at the end of the long-term shape run. These cells experienced moderate net deposition (Figures 3b and 4b) of higher concentration sediments. The initial vertical profiles were shifted downward and the concentrations in the upper 15 cm reflect the time history of CFT model dynamics (e.g., erosion, deposition, mixing).

Steps 3 & 4: Interpolated initial bed concentrations for the model run.

Conclusion: The algorithm is working as designed and the shape is being driven by the time history of CFT model dynamics during the shape run.

Figures 1e and 1f of USEPA Attachment 4

The steps to create concentration profiles for grid cells [17, 235] and [17, 233] are shown in Figures 5a and 6a of these notes and the bed thickness changes for the same cells are shown in Figures 5b and 6b. The profiles reflect:

Step 0: Raw IC derived from the mapping of sediment core data for each data interval (converted to volumetric concentration using model bulk density).

Step 1: Subsurface IC for the "shape run". The change in concentration between the 0 to 15 cm and 15 to 45 cm intervals was here too large for the interpolation function (Appendix O, Section 3.1.2) to accommodate and consequently the raw IC concentration values remained unchanged.

Step 2: The concentration profile at the end of the long-term shape run. These cells experienced large deposition events[3] (Figures 5b and 6b) and the 0 to 15 cm initial concentrations were fully buried by sediments with lower concentrations. The final shape in the upper 0 to 15 cm also reflects the time history of more gradual CFT dynamics over the remainder of the run.

Steps 3 & 4: Interpolated initial bed concentrations for the model run.

Conclusion: The algorithm is working as designed and the shape is being driven by large deposition events followed by more gradual CFT dynamics during the shape run.

[3] It is noted that the deposition event in cell [17, 235] (Figure 5b) coincides with an erosion event in the adjacent upstream cell [17, 236] discussed previously (Figure 1b). Likewise, the deposition event in cell [17, 233] (Figure 6b) coincides with the erosion event in the adjacent upstream cell [17, 234] shown in Figure 2b.

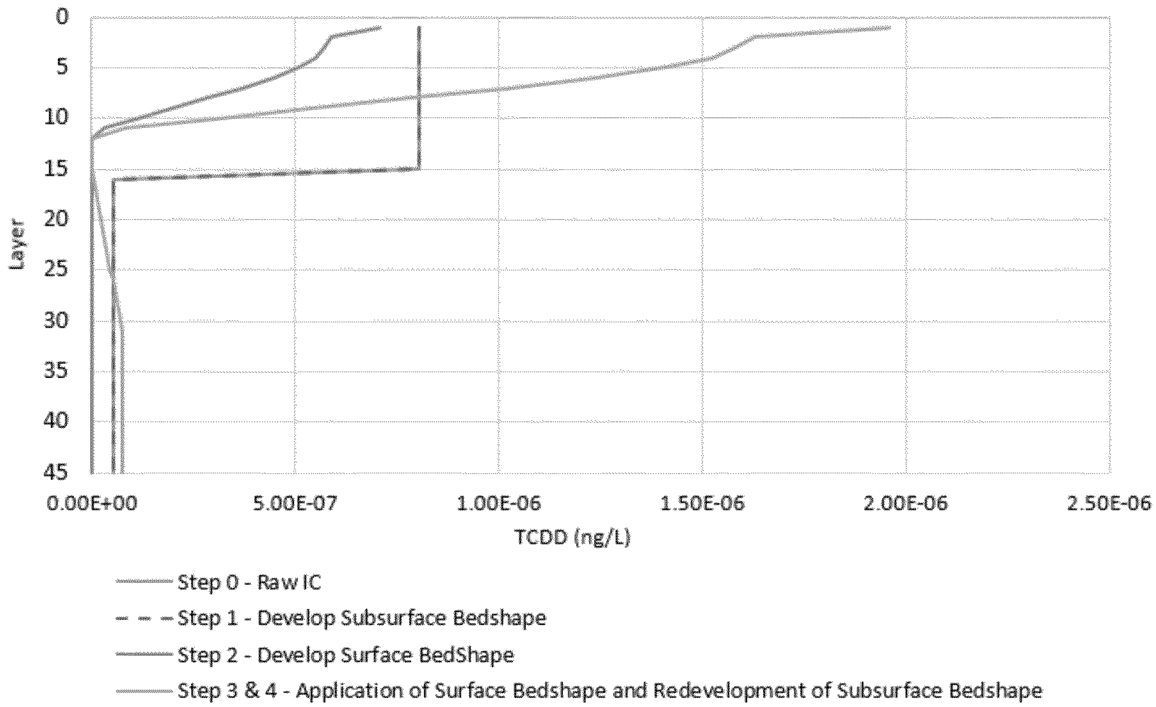

Figure 1a. Initial Sediment 2,3,7,8-TCDD Concentration Profile Development for Cell [17, 236]

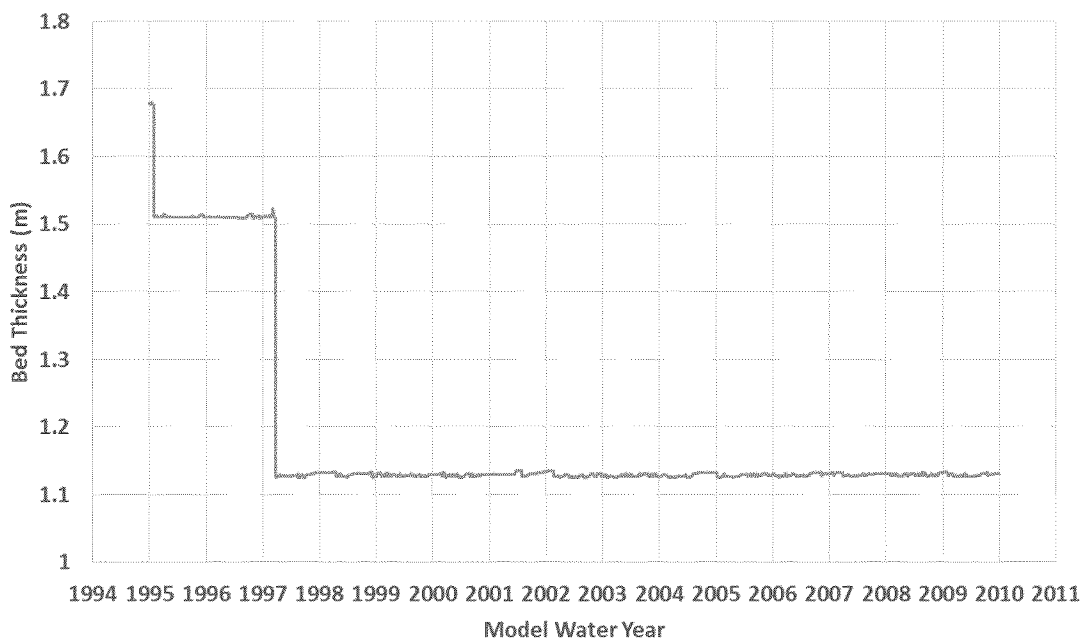

Figure 1b. CFT Model Bed Thickness During Long-term Calibration Shape Run for Cell [17, 236]

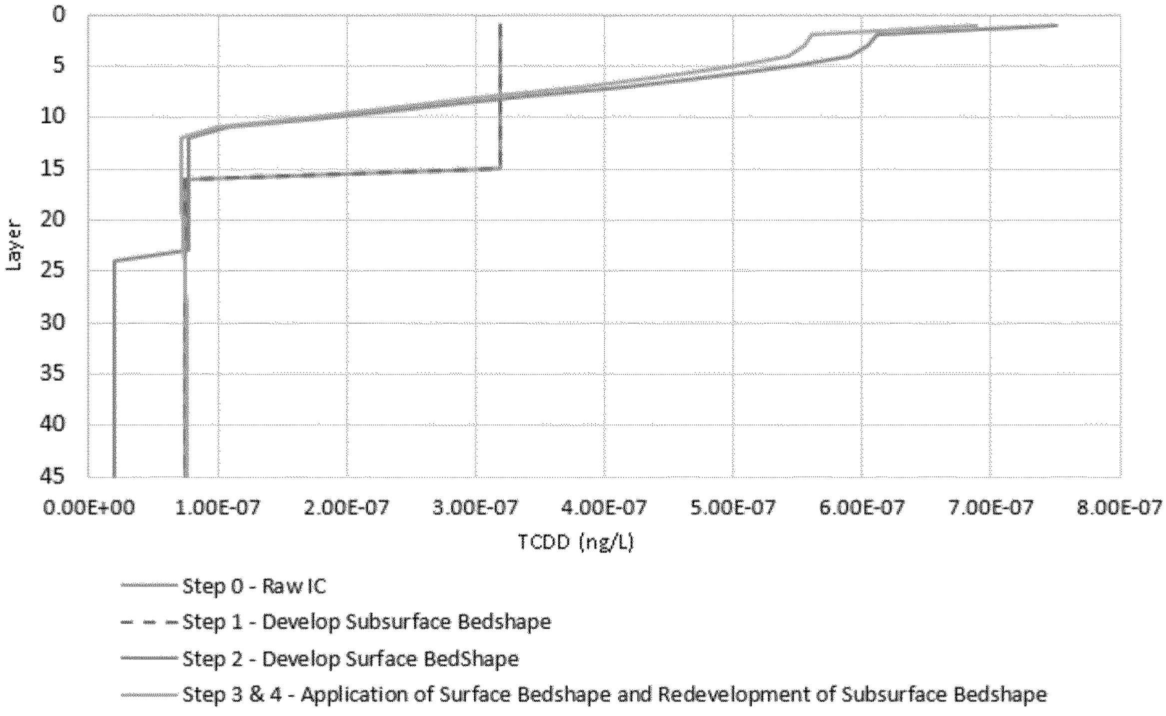

Figure 2a. Initial Sediment 2,3,7,8-TCDD Concentration Profile Development for Cell [17, 234]

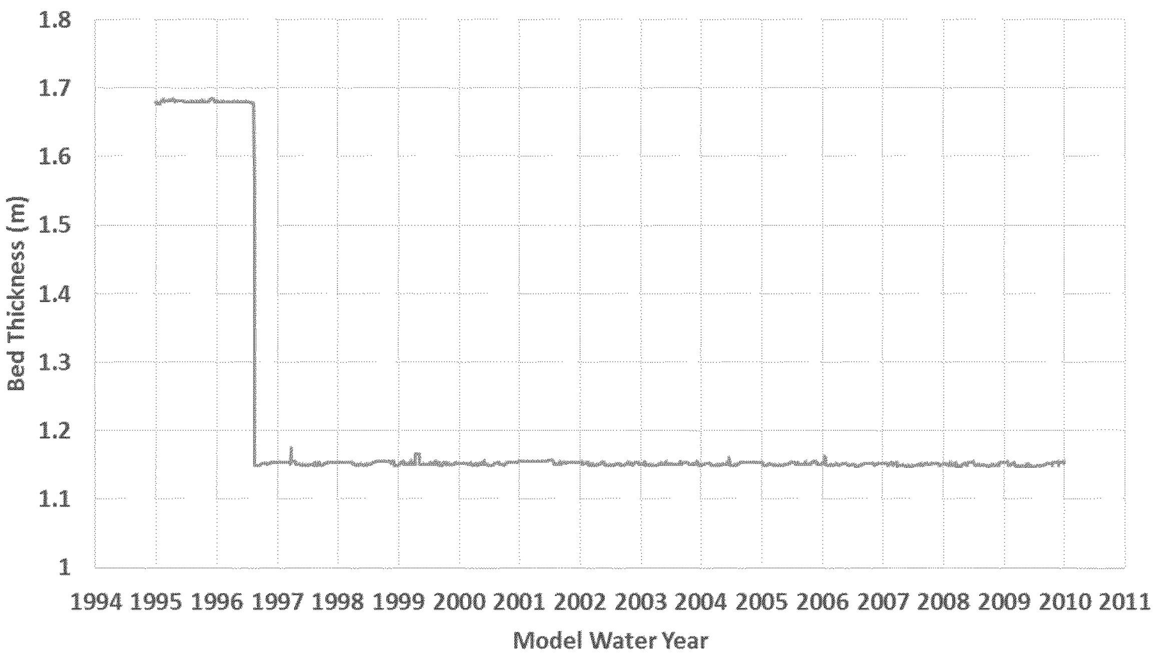

Figure 2b. CFT Model Bed Thickness During Long-term Calibration Shape Run for Cell [17, 234]

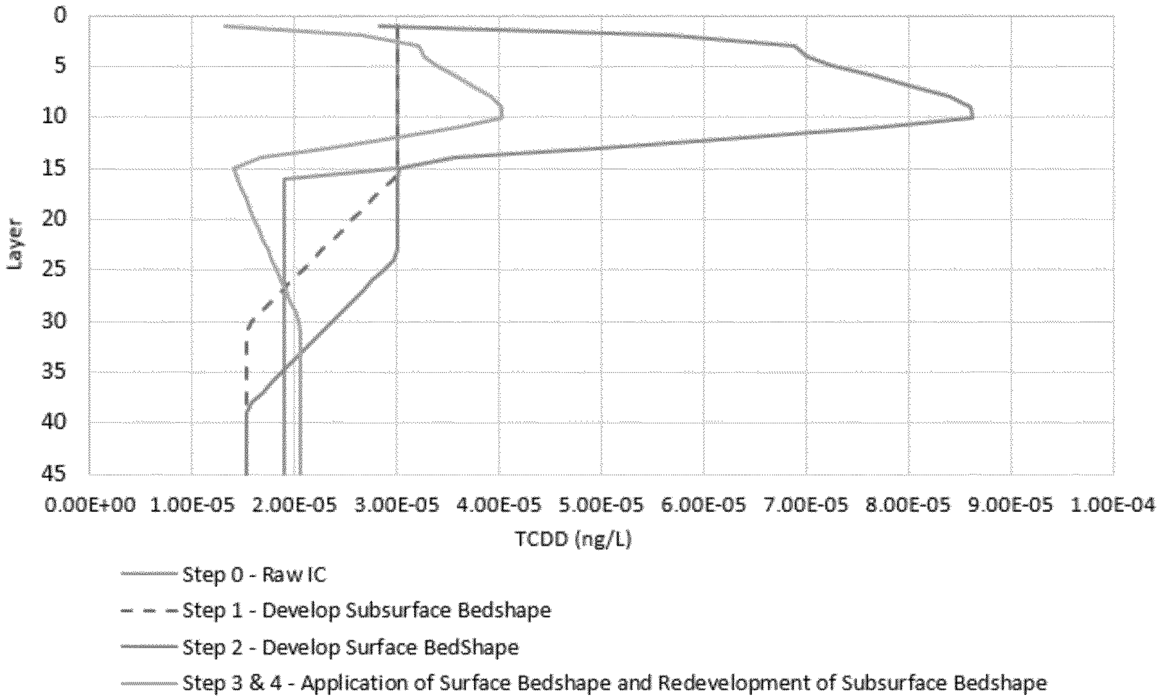

Figure 3a. Initial Sediment 2,3,7,8-TCDD Concentration Profile Development for Cell [18, 90]

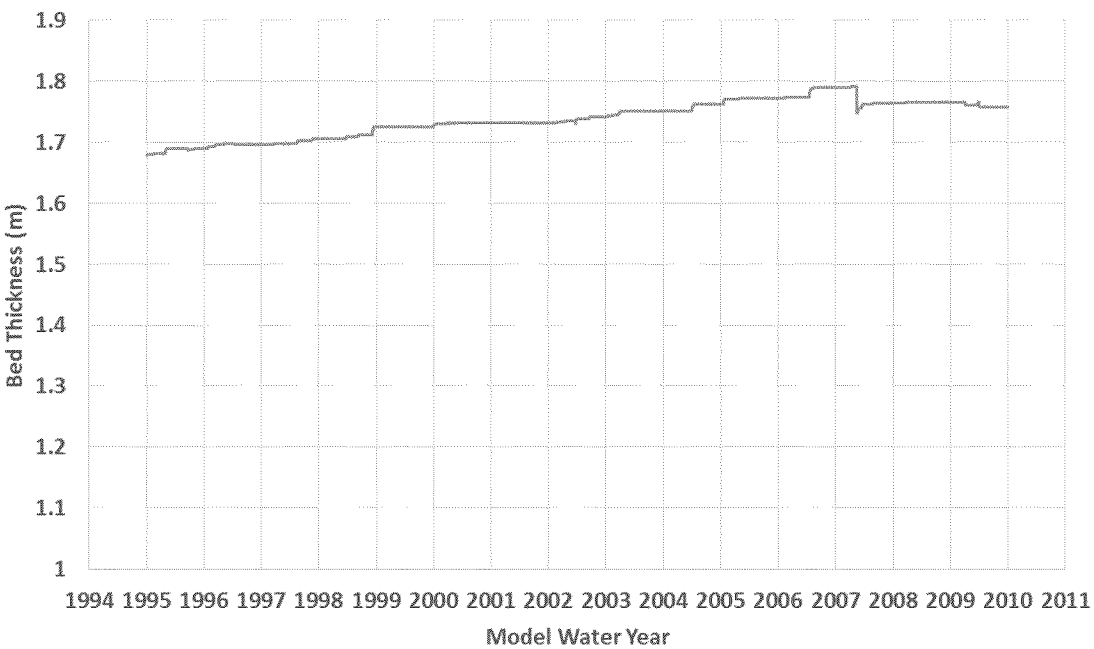

Figure 3b. CFT Model Bed Thickness During Long-term Calibration Shape Run for Cell [18, 90]

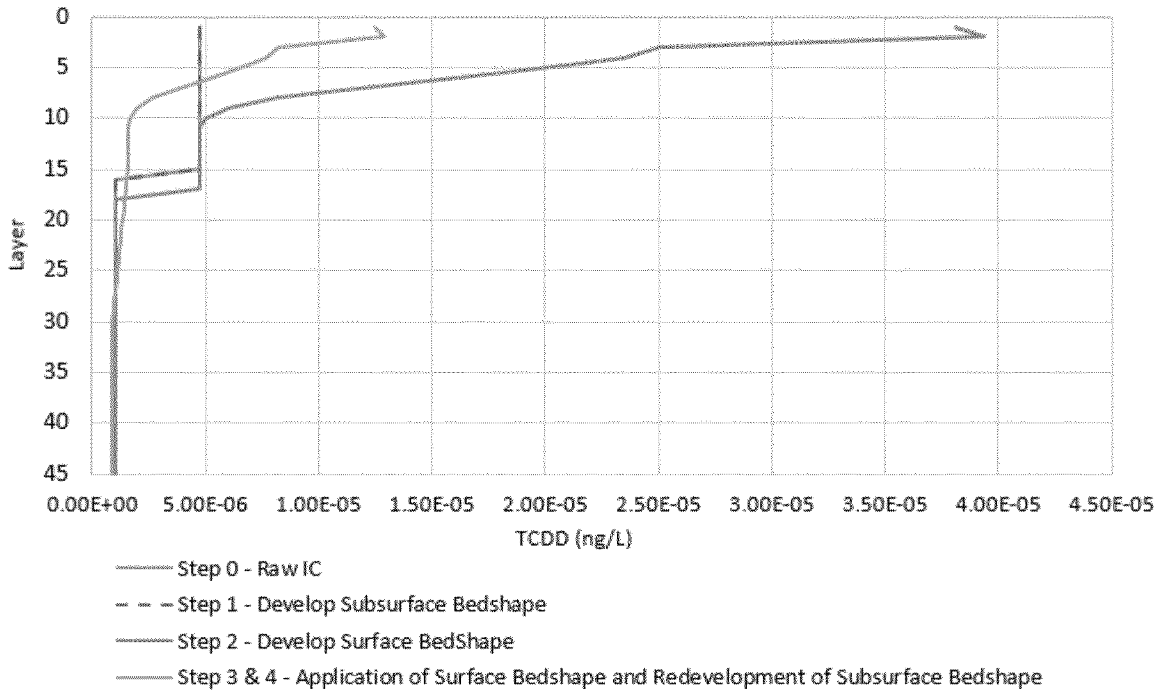

Figure 4a. Initial Sediment 2,3,7,8-TCDD Concentration Profile Development for Cell [22, 94]

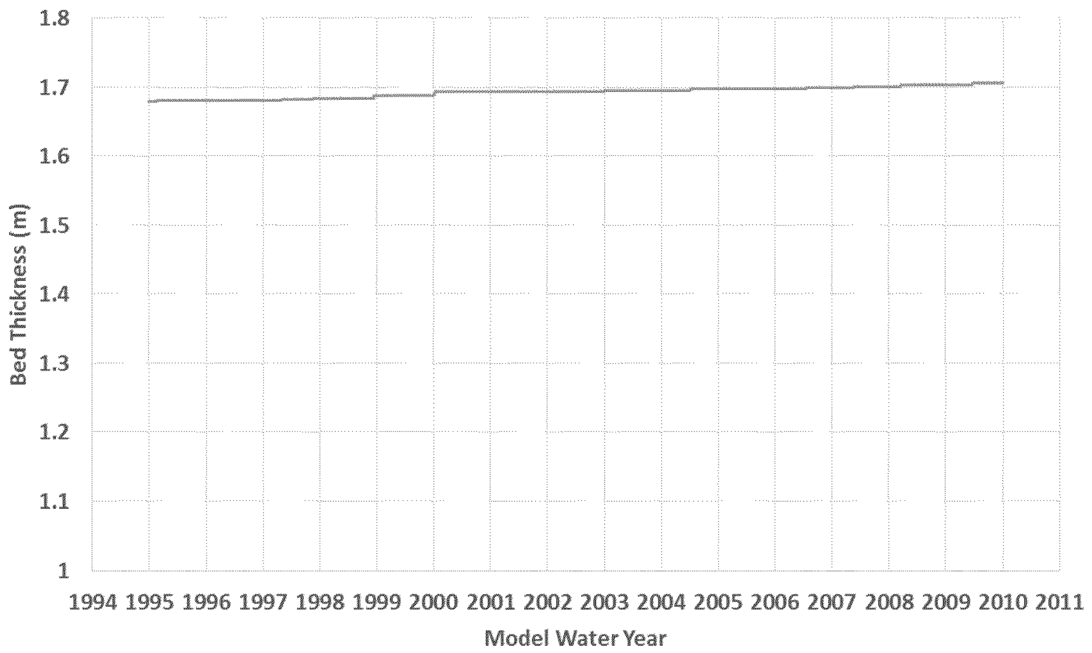

Figure 4b. CFT Model Bed Thickness During Long-term Calibration Shape Run for Cell [22, 94]

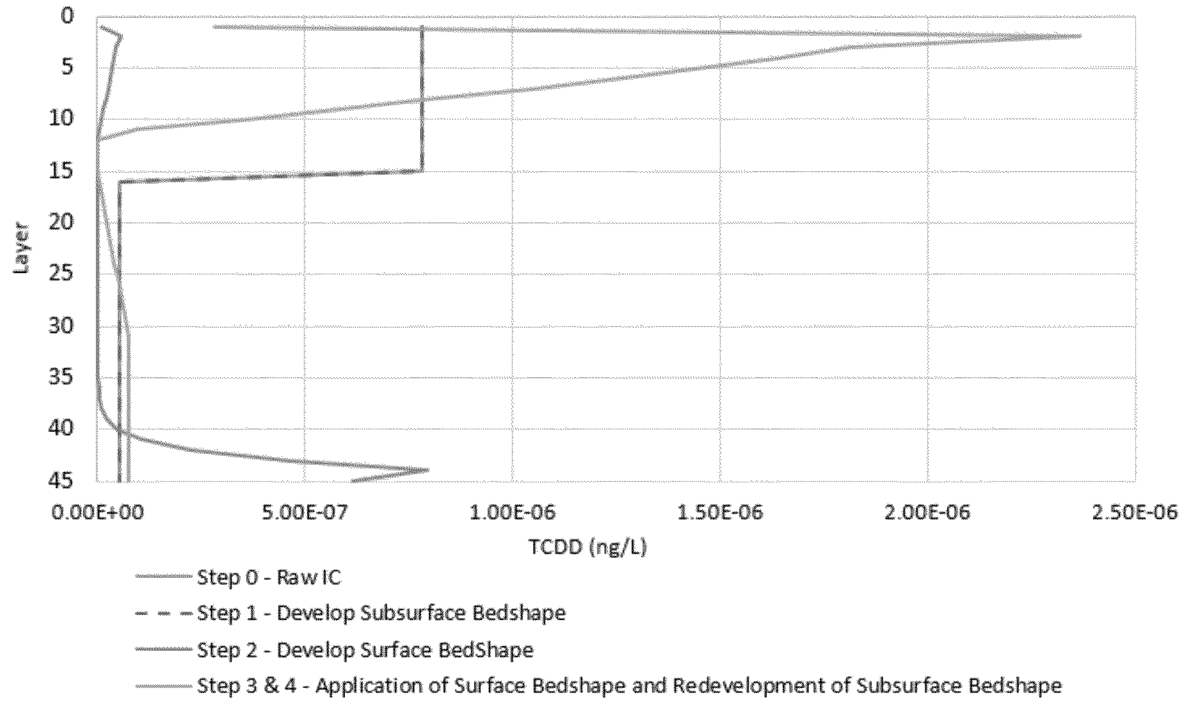

Figure 5a. Initial Sediment 2,3,7,8-TCDD Concentration Profile Development for Cell [17, 235]

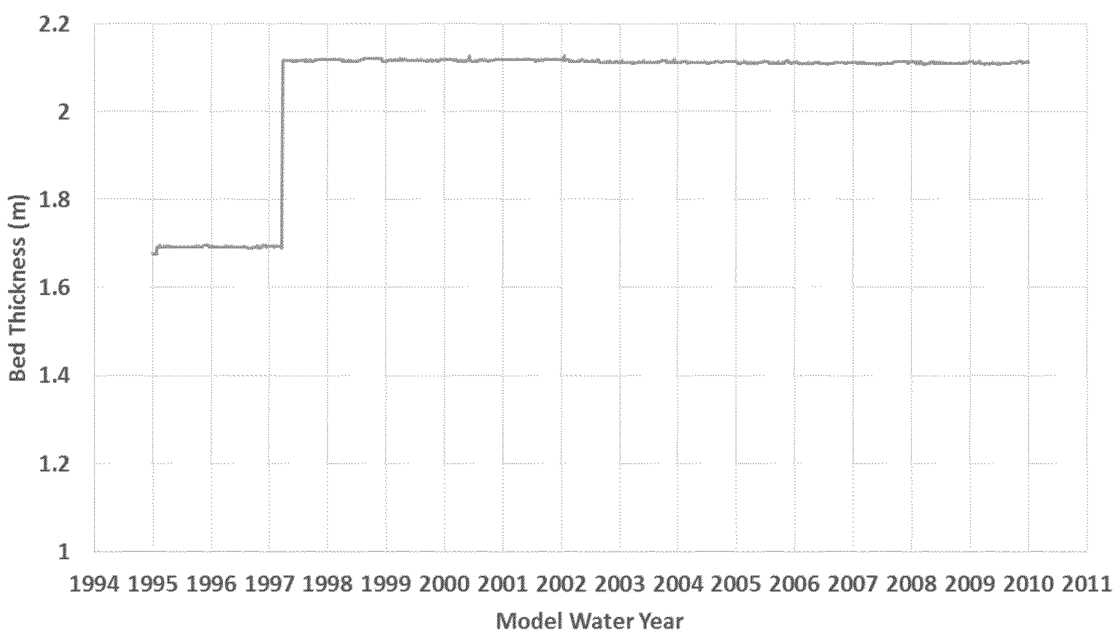

Figure 5b. CFT Model Bed Thickness During Long-term Calibration Shape Run for Cell [17, 235]

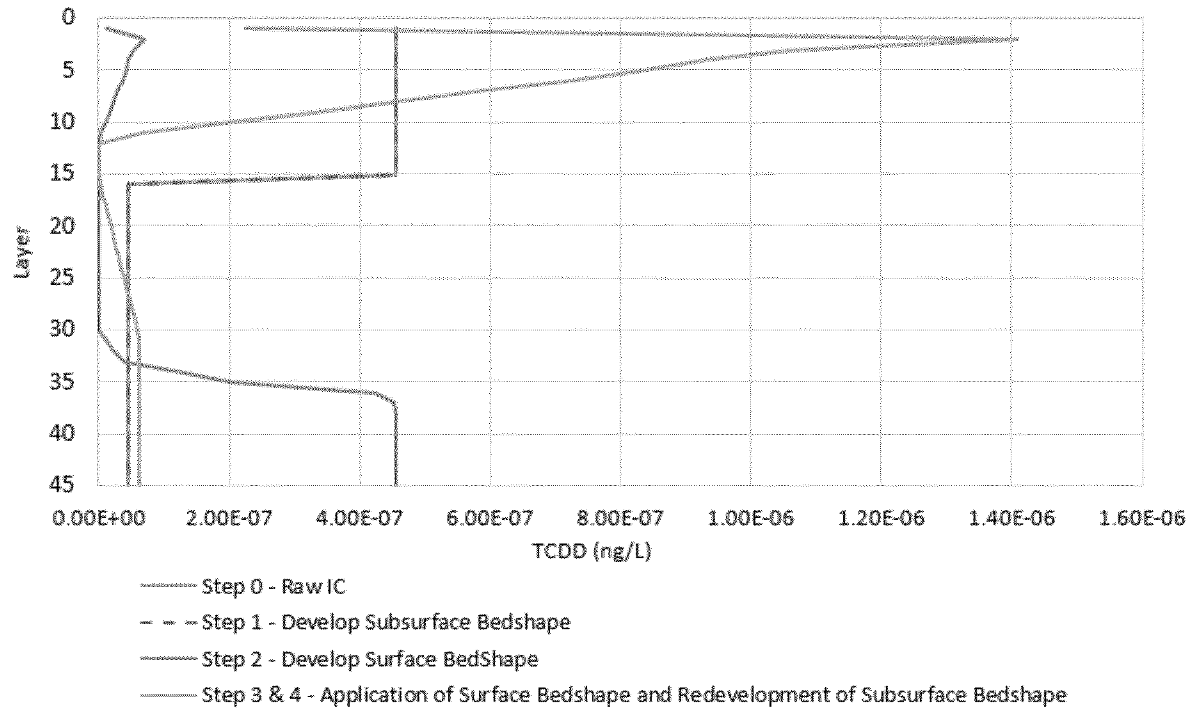

Figure 6a. Initial Sediment 2,3,7,8-TCDD Concentration Profile Development for Cell [17, 233]

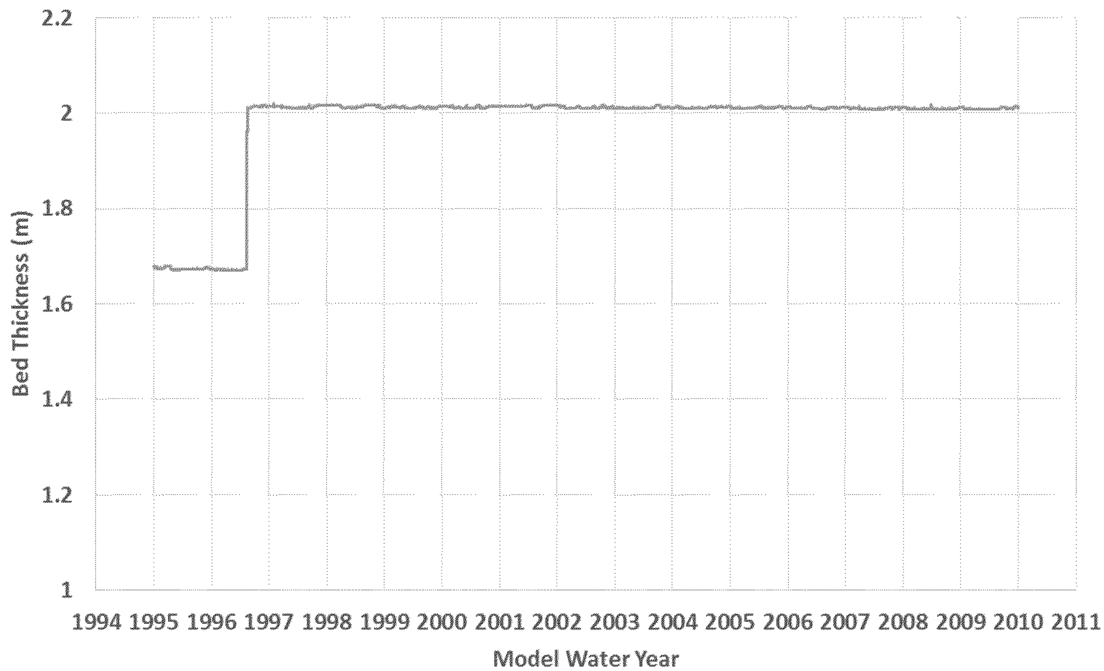

Figure 6b. CFT Model Bed Thickness During Long-term Calibration Shape Run for Cell [17, 233]